

This worksheet calculates the transient advection, dispersion, and decay of PCE in the vadose zone. PCE is transported in both the aqueous and vapor phases. Local thermodynamic equilibrium is assumed so that the partitioning of tritium between the aqueous and gas phases can be expressed using Henry's Law. The half-life of PCE ranges from 9 months (EPA fact sheet) to infinity. This solution is derived in Jury et al., 1983, J. Env. Qual., 12, 558-564 and in Jury et al., 1990, WRR, 26(1), 13-20.

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9/26/05

Input parameters and distributions:

Define number of realizations: $n := 100$ Molecular weight of PCE: MW := 165.83

$i := 1..n$

Total porosity: $\phi := \text{runif}(n, .302, .445)$ median(ϕ) = 0.378

Moisture Content: $\theta_w := \text{runif}(n, .053, .225)$

Gas Content: $a := \phi - \theta_w$ max(a) = 0.38

Henry's Constant: $K_H := 0.42$ This is Cg/Cliq

(EPA online calculator: www.epa.gov/athens/learn2model/part-two/onsite/esthenry.htm)

Adsorption partition coefficient: $\log K_d := \text{runif}(n, -1.4, .3)$ $K_{d_i} := \frac{10^{\log K_{d_i}}}{1000} \cdot m^3 \cdot kg^{-1}$

Liquid-Phase Diffusion Coefficient: $D_w := 9.2 \cdot 10^{-10} \cdot \frac{m^2}{s}$ See Reid et al. (1987), pp. 587, 598

Gas-Phase Diffusion Coefficient: $D_g := 9.5 \cdot 10^{-6} \cdot \frac{m^2}{s}$

Half-life: $\log_t_{half} := \text{runif}(n, 7.4, 17.5)$

$t_{half_i} := 10^{\log_t_{half_i}} \cdot s$ median(t_{half}) = $4.202 \times 10^{12} s$

min(t_{half}) = $2.563 \times 10^7 s$

Bulk density: $\rho_b := \text{runif}(n, 1470, 1850) \cdot kg \cdot m^{-3}$ median(ρ_b) = $1.691 \times 10^3 kg m^{-3}$

Gas Concentration: ppb := $\text{runif}(n, 5900, 5900 \cdot 10)$

Waste zone length: $\text{length} := 430 \cdot .3048 \cdot \text{m}$

Waste zone width: $\text{width} := 300 \cdot .3048 \cdot \text{m}$

Minimum length and width is determined by size of pit 33 (10'x10')

Maximum length and width is determined by extent of MWL.

Waste zone thickness: $L := \text{runif}(n, 10 \cdot .3048, 27 \cdot .3048) \cdot \text{m}$ $\text{mean}(L) = 5.697 \text{ m}$

Distance to water table: $d_{\text{wt}} := \text{runif}(n, 461 \cdot .3048, 495 \cdot .3048) \cdot \text{m}$

Thickness of clean overburden: $L_c := \text{runif}(n, 0 \cdot .3048, 16 \cdot .3048) \cdot \text{m}$

6 to 16 feet nominal; 0 minimum is due to erosion

Darcy Infiltration: $q := \text{runif}(n, 1.18 \cdot 10^{-11}, 6.12 \cdot 10^{-11}) \cdot \frac{\text{m}}{\text{s}}$

Surface boundary-layer thickness: $d_{\text{BL}} := \text{runif}(n, 0.001, 1) \cdot \text{m}$

Tortuosity Factor: $\varepsilon_w := \text{runif}(n, 0.001, 1)$

(lower bound from Millington 1959; upper bound is physical limit) $\varepsilon_g := \text{runif}(n, 0.1, 1)$

US Environmental Protection Agency. 1988. Federal guidance report no. 11: limiting values of radionuclide intake and air concentration and dose conversion factors for inhalation, submersion, and ingestion, Eckerman, K.F., A.B. Wolbarst, and A.C.B. Richardson, Washington, DC: US Environmental Protection Agency. Report No.: EPA-5201/1-88-020.

Input Parameter Distributions for sensitivity analyses:

$$K_d = \begin{array}{|c|c|} \hline & 1 \\ \hline 1 & 3.327 \cdot 10^{-4} \\ \hline \end{array} \text{ m}^3 \text{ kg}^{-1} \quad \phi = \begin{array}{|c|c|} \hline & 1 \\ \hline 1 & 0.302 \\ \hline \end{array}$$

$$L = \begin{array}{|c|c|} \hline & 1 \\ \hline 1 & 5.184 \\ \hline \end{array} \text{ m}$$

$$\theta_w = \begin{array}{|c|c|} \hline & 1 \\ \hline 1 & 0.128 \\ \hline \end{array}$$

$$L_c = \begin{array}{|c|c|} \hline & 1 \\ \hline 1 & 0.364 \\ \hline \end{array} \text{ m} \quad q = \begin{array}{|c|c|} \hline & 1 \\ \hline 1 & 1.915 \cdot 10^{-11} \\ \hline \end{array} \text{ m s}^{-1}$$

$$d_{\text{wt}} = \begin{array}{|c|c|} \hline & 1 \\ \hline 1 & 146.778 \\ \hline \end{array} \text{ m}$$

$$d_{\text{BL}} = \begin{array}{|c|c|} \hline & 1 \\ \hline 1 & 0.05 \\ \hline \end{array} \text{ m}$$

$$\varepsilon_w = \begin{array}{|c|c|} \hline & 1 \\ \hline 1 & 0.773 \\ \hline \end{array}$$

$$\varepsilon_g = \begin{array}{|c|c|} \hline & 1 \\ \hline 1 & 0.637 \\ \hline \end{array}$$

$$t_{\text{half}} = \begin{array}{|c|c|} \hline & 1 \\ \hline 1 & 5.269 \cdot 10^{14} \\ \hline 2 & 2.568 \cdot 10^{14} \\ \hline \end{array} \text{ s}$$

$$\text{ppb} = \begin{array}{|c|c|} \hline & 1 \\ \hline 1 & 4.911 \cdot 10^4 \\ \hline \end{array}$$

Calculated Parameters

Volume of waste zone:

$$V_i := \text{length} \cdot \text{width} \cdot L_i$$

$$C_{\text{gas}_i} := \frac{\text{ppb}_i}{10^9} \cdot 0.8 \quad \text{partial pressure of PCE in atmospheres (where 0.8 is the atmospheric pressure in Albuquerque)}$$

$$C_{o_i} := \frac{C_{\text{gas}_i}}{0.01} \cdot \frac{\text{MW}}{1000} \cdot \text{kg} \cdot \text{m}^{-3}$$

max(C_{gas}) = 4.717×10^{-5} 0.01 is Henry's constant in atm-m³/mol
 max(C_o) = 7.822×10^{-4} kg m⁻³

$$\text{inventory}_i := C_{o_i} \cdot V_i$$

$$\text{max}(\text{inventory}) = 69.564 \text{ kg}$$

$$\text{min}(\text{inventory}) = 5.041 \text{ kg}$$

Retardation factor:

$$R_{L_i} := \rho_{b_i} \cdot K_{d_i} + \theta_{w_i} + a_i \cdot K_H$$

Effective Diffusion Coefficient:

$$D_{E_i} := \frac{(\varepsilon_{w_i} \cdot D_w + \varepsilon_{g_i} \cdot K_H \cdot D_g)}{R_{L_i}}$$

Effective Velocity:

$$V_{E_i} := \frac{q_i}{R_{L_i}}$$

Decay constant:

$$\mu_i := \frac{\ln(2)}{t_{\text{half}_i}}$$

$$\mu = \begin{array}{|c|c|} \hline & 1 \\ \hline 1 & 1.316 \cdot 10^{-15} \text{ s}^{-1} \\ \hline 2 & 2.699 \cdot 10^{-15} \\ \hline \end{array}$$

Surface mass-transfer coefficient:

$$H_{E_i} := \frac{D_g}{d_{BL_i}} \cdot \frac{K_H}{R_{L_i}}$$

$$\text{Note: } R_L / K_H = R_G$$

Concentration at water table as a function of time:

$$\text{ntimes} := 100$$

$$\text{nyears} := 1000$$

$$j := 1 .. \text{ntimes}$$

$$\text{nsec} := \text{nyears} \cdot 365.25 \cdot 24 \cdot 3600$$

The d_{wt} parameter can be assigned a constant value ($d_{wt,i}$) to simulate concentrations at different depths.

Time:

$$t_j := \frac{j}{\text{ntimes}} \cdot \text{nsec} \cdot \text{s}$$

$$\text{erfc}(x) := 1 - \text{erf}(x)$$

$$d_{wt} = \begin{array}{|c|c|} \hline & 1 \\ \hline 1 & 146.778 \\ \hline 2 & 144.257 \\ \hline \end{array} \text{ m}$$

Parameters for system with clean overburden plus source thickness

$$\text{exp1}_{i,j} := \text{if} \left[\frac{\left[H_{E_i} \cdot (H_{E_i} + V_{E_i}) \cdot t_j + (H_{E_i} + V_{E_i}) \cdot d_{wt_i} \right]}{D_{E_i}} > 700, 700, \frac{\left[H_{E_i} \cdot (H_{E_i} + V_{E_i}) \cdot t_j + (H_{E_i} + V_{E_i}) \cdot d_{wt_i} \right]}{D_{E_i}} \right]$$

$$\text{exp2}_i := \text{if} \left[\frac{H_{E_i} \cdot (L_i + L_{c_i})}{D_{E_i}} > 700, 700, \frac{H_{E_i} \cdot (L_i + L_{c_i})}{D_{E_i}} \right] \quad \text{exp3}_i := \text{if} \left(\frac{V_{E_i} \cdot d_{wt_i}}{D_{E_i}} > 700, 700, \frac{V_{E_i} \cdot d_{wt_i}}{D_{E_i}} \right)$$

$$A1_{i,j} := \text{erfc} \left(\frac{d_{wt_i} - (L_i + L_{c_i}) - V_{E_i} \cdot t_j}{\sqrt{4 \cdot D_{E_i} \cdot t_j}} \right) \quad A2_{i,j} := \text{erfc} \left(\frac{d_{wt_i} - V_{E_i} \cdot t_j}{\sqrt{4 \cdot D_{E_i} \cdot t_j}} \right)$$

$$A4_{i,j} := \text{erfc} \left(\frac{d_{wt_i} + V_{E_i} \cdot t_j}{\sqrt{4 \cdot D_{E_i} \cdot t_j}} \right) \quad A5_{i,j} := \exp(\text{exp1}_{i,j}) \quad A3_{i,j} := \text{erfc} \left(\frac{d_{wt_i} + (L_i + L_{c_i}) + V_{E_i} \cdot t_j}{\sqrt{4 \cdot D_{E_i} \cdot t_j}} \right)$$

$$A6_{i,j} := \text{erfc} \left(\frac{d_{wt_i} + (2 \cdot H_{E_i} + V_{E_i}) \cdot t_j}{\sqrt{4 \cdot D_{E_i} \cdot t_j}} \right) \quad A7_{i,j} := \text{erfc} \left(\frac{d_{wt_i} + (L_i + L_{c_i}) + (2 \cdot H_{E_i} + V_{E_i}) \cdot t_j}{\sqrt{4 \cdot D_{E_i} \cdot t_j}} \right)$$

Parameters for clean overburden alone:

$$\text{exp2c}_i := \text{if} \left(\frac{H_{E_i} \cdot L_{c_i}}{D_{E_i}} > 700, 700, \frac{H_{E_i} \cdot L_{c_i}}{D_{E_i}} \right)$$

$$A1c_{i,j} := \text{erfc} \left(\frac{d_{wt_i} - L_{c_i} - V_{E_i} \cdot t_j}{\sqrt{4 \cdot D_{E_i} \cdot t_j}} \right)$$

$$A3c_{i,j} := \text{erfc} \left(\frac{d_{wt_i} + L_{c_i} + V_{E_i} \cdot t_j}{\sqrt{4 \cdot D_{E_i} \cdot t_j}} \right)$$

$$A7c_{i,j} := \operatorname{erfc}\left[\frac{d_{wt_i} + L_{c_i} + (2 \cdot H_{E_i} + V_{E_i}) \cdot t_j}{\sqrt{4 \cdot D_{E_i} \cdot t_j}}\right]$$

Concentration with just clean overburden:

$$C_{Tc_{i,j}} := 0.5 \cdot C_{o_i} \cdot \exp(-\mu_i \cdot t_j) \cdot \left[A1c_{i,j} - A2_{i,j} + \left(1 + \frac{V_{E_i}}{H_{E_i}} \right) \cdot \exp(\exp3_i) \cdot (A3c_{i,j} - A4_{i,j}) \dots \right. \\ \left. + \left(2 + \frac{V_{E_i}}{H_{E_i}} \right) \cdot A5_{i,j} \cdot (A6_{i,j} - \exp(\exp2_i) \cdot A7_{i,j}) \right]$$

Concentration with clean overburden plus source thickness:

$$C_{Tt_{i,j}} := 0.5 \cdot C_{o_i} \cdot \exp(-\mu_i \cdot t_j) \cdot \left[A1_{i,j} - A2_{i,j} + \left(1 + \frac{V_{E_i}}{H_{E_i}} \right) \cdot \exp(\exp3_i) \cdot (A3_{i,j} - A4_{i,j}) \dots \right. \\ \left. + \left(2 + \frac{V_{E_i}}{H_{E_i}} \right) \cdot A5_{i,j} \cdot (A6_{i,j} - \exp(\exp2_i) \cdot A7_{i,j}) \right]$$

Combined concentration using superposition (Jury et al., 1990, WRR, 26(1), 13-20).

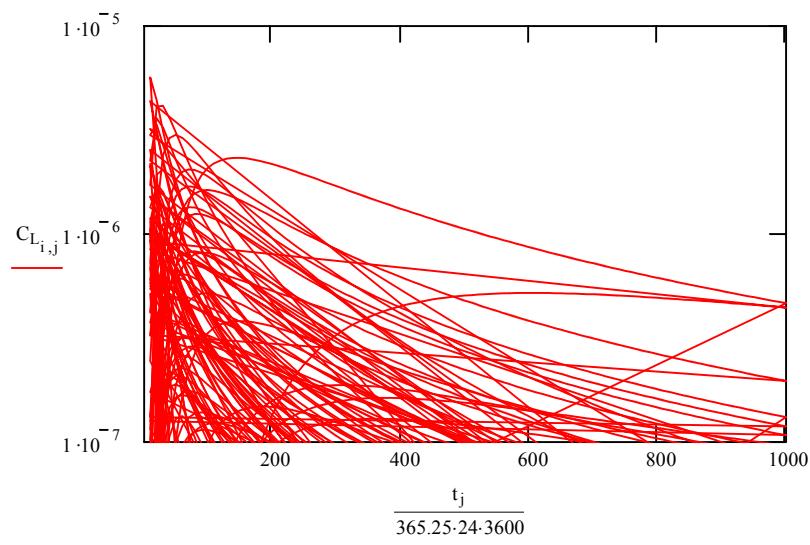
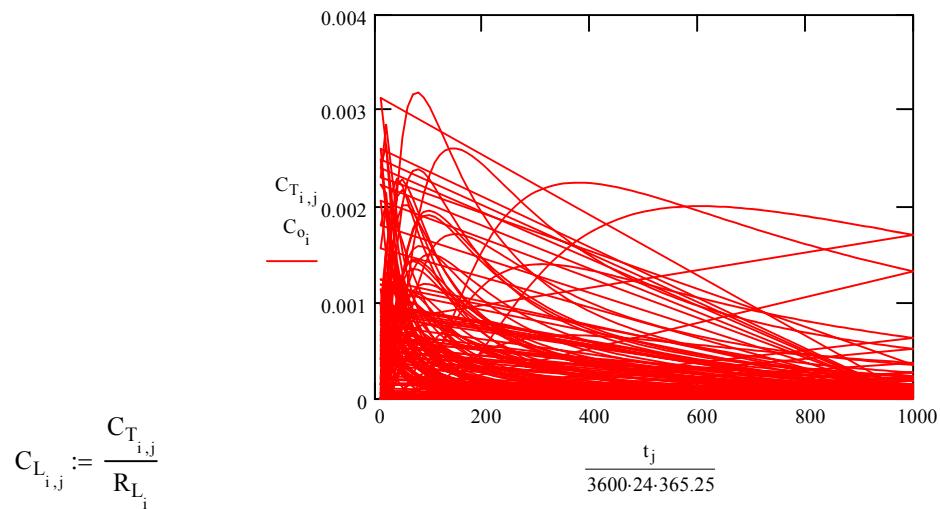
$$C_{Ti,j} := C_{Tt_{i,j}} - C_{Tc_{i,j}}$$

$$\max(C_T) = 1.732 \times 10^{-6} \text{ kg m}^{-3}$$

$$C_{Ti,j} := \operatorname{if}(C_{Tt_{i,j}} < 0, 0, C_{Tt_{i,j}})$$

$$\max(C_{Ti}) = 1.987 \times 10^{-6} \text{ kg m}^{-3}$$

$$\max(C_{Tc}) = 3.323 \times 10^{-7} \text{ kg m}^{-3}$$



$$\max(C_L) = 5.639 \times 10^{-6} \text{ kg m}^{-3}$$

$$\text{median}(C_L) = 2.868 \times 10^{-8} \text{ kg m}^{-3}$$

$$C_{L_{\mu g L_{i,j}}} := C_{L_{i,j}} \cdot 10^6$$

$$\max(C_{L_{\mu g L}}) = 5.639 \text{ kg m}^{-3}$$

This is the concentration in ppb

$$t_j := \frac{j}{\text{ntimes}} \cdot 10 \cdot 3600 \cdot 24 \cdot 365.25 \cdot s$$

0.134	0.504
4.349	3.161
2.243 \cdot 10^{-3}	0.176

Calculate surface flux as a function of time

$C_{L,\mu g,L}$

Parameters for source plus clean overburden:

$$J1_{i,j} := \operatorname{erfc}\left(\frac{V_{E_i} \cdot t_j}{\sqrt{4 \cdot D_{E_i} \cdot t_j}}\right) \quad J2_{i,j} := \operatorname{erfc}\left(\frac{L_i + L_{c_i} + V_{E_i} \cdot t_j}{\sqrt{4 \cdot D_{E_i} \cdot t_j}}\right)$$

$$J3_{i,j} := \operatorname{if}\left[\frac{H_{E_i} \cdot (H_{E_i} + V_{E_i}) \cdot t_j}{D_{E_i}} > 700, 700, \frac{H_{E_i} \cdot (H_{E_i} + V_{E_i}) \cdot t_j}{D_{E_i}}\right]$$

$$J4_i := \operatorname{if}\left[\frac{H_{E_i} \cdot (L_i + L_{c_i})}{D_{E_i}} > 700, 700, \frac{H_{E_i} \cdot (L_i + L_{c_i})}{D_{E_i}}\right]$$

$$J5_{i,j} := \operatorname{erfc}\left[\frac{(L_i + L_{c_i}) + (2 \cdot H_{E_i} + V_{E_i}) \cdot t_j}{\sqrt{4 \cdot D_{E_i} \cdot t_j}}\right] \quad J6_{i,j} := \operatorname{erfc}\left[\frac{(2 \cdot H_{E_i} + V_{E_i}) \cdot t_j}{\sqrt{4 \cdot D_{E_i} \cdot t_j}}\right]$$

Parameters for clean overburden only:

$$J2c_{i,j} := \operatorname{erfc}\left(\frac{L_{c_i} + V_{E_i} \cdot t_j}{\sqrt{4 \cdot D_{E_i} \cdot t_j}}\right)$$

$$J4c_i := \operatorname{if}\left[\frac{H_{E_i} \cdot (L_{c_i})}{D_{E_i}} > 700, 700, \frac{H_{E_i} \cdot (L_{c_i})}{D_{E_i}}\right]$$

$$J5c_{i,j} := \operatorname{erfc}\left[\frac{(L_{c_i}) + (2 \cdot H_{E_i} + V_{E_i}) \cdot t_j}{\sqrt{4 \cdot D_{E_i} \cdot t_j}}\right]$$

Surface flux with both source and clean overburden:

$$J_{st,i,j} := 0.5 \cdot C_{o_i} \cdot \exp(-\mu_i \cdot t_j) \cdot [V_{E_i} \cdot (J1_{i,j} - J2_{i,j}) + (2 \cdot H_{E_i} + V_{E_i}) \cdot \exp(J3_{i,j}) \cdot (\exp(J4_i) \cdot J5_{i,j} - J6_{i,j})]$$

Surface flux with just clean overburden:

$$J_{sc,i,j} := 0.5 \cdot C_{o_i} \cdot \exp(-\mu_i \cdot t_j) \cdot [V_{E_i} \cdot (J1_{i,j} - J2_{c_i,j}) + (2 \cdot H_{E_i} + V_{E_i}) \cdot \exp(J3_{i,j}) \cdot (\exp(J4_{c_i}) \cdot J5_{c_i,j} - J6_{i,j})]$$

Combined concentration using superposition (Jury et al., 1990, WRR, 26(1), 13-20).

$$J_{s,i,j} := J_{st,i,j} - J_{sc,i,j}$$

This is the downward total flux at the surface. The volatilization flux is equal to the negative of this value.

$$J_{s,i,j} := \text{if}(J_{s,i,j} > 0, 0, -J_{s,i,j})$$

$$\text{mean}(J_{st}) = -5.018 \times 10^{-13} \text{ kg m}^{-2} \text{ s}^{-1}$$

$$\text{mean}(J_{sc}) = -1.951 \times 10^{-13} \text{ kg m}^{-2} \text{ s}^{-1}$$

$$\max(J_s) = 3.694 \times 10^{-10} \text{ kg m}^{-2} \text{ s}^{-1}$$

$$J_{s_ng_m2_min}_{i,j} := J_{s,i,j} \cdot 10^{12} \cdot 60 \quad \text{Surface flux in ng/m}^2/\text{min}$$

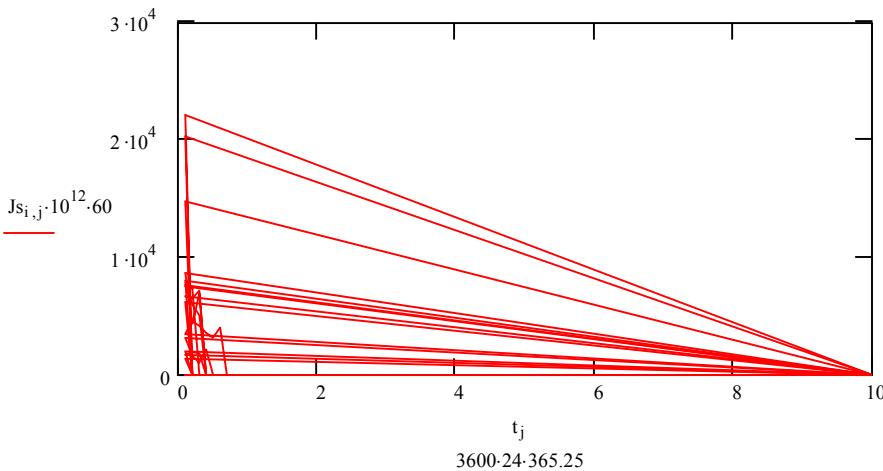
$$\min(J_s) = 0 \text{ kg m}^{-2} \text{ s}^{-1}$$

$$\max(J_{s_ng_m2_min}) = 2.216 \times 10^4 \text{ kg m}^{-2} \text{ s}^{-1}$$

0	0
0	0
0	0

$$J_{s_ng_m2_min}$$

This is the surface volatilization flux to the atmosphere



Calculate atmospheric concentration and dose to an individual inhaling the air directly above the waste site.

$$\text{Average wind speed (m/s): } v_{\text{wind}} := 3.63 \cdot m \cdot s^{-1}$$

(from average of SNL Site Environmental Monitoring Reports 1990-1996)

$$\text{Vertical atmospheric mixing length (m): } L_v := 2 \cdot m$$

(conservative value to encompass volume most likely occupied by the average human, Yu, C. et al., 1993, Data Collection Handbook to Support Modeling the Impacts of Radioactive Material in Soil, ANL/EAIS-8, Argonne National Laboratory, Argonne, Illinois.)

$$\text{length} = 131.064 \text{ m} \quad \text{width} = 91.44 \text{ m}$$

$$\text{Lateral atmospheric mixing distance (m): } L_h := \text{if}(length < width, length, width)$$

(the lateral atmospheric mixing distance is conservatively estimated as the minimum of either the length or width of the waste zone)

$$L_h = 91.44 \text{ m}$$

$$\text{Flow rate of air in mixing volume: } Q_{\text{wind}} := v_{\text{wind}} \cdot L_v \cdot L_h$$

$$\text{PCE concentration in atmosphere (kg/m}^3\text{: } C_{\text{atm}_{i,j}} := \frac{J s_{i,j} \cdot \text{length} \cdot \text{width}}{Q_{\text{wind}}}$$

$$\max(C_{\text{atm}}) = 6.669 \times 10^{-9} \text{ kg m}^{-3}$$

$$\text{Inhalation rate: } I := \frac{20}{24 \cdot 3600} \cdot m^3 \cdot s^{-1} \quad I = 2.315 \times 10^{-4} \text{ m}^3 \text{ s}^{-1}$$

(20 m³/day from U.S. EPA 1991, U.S. Environmental Protection Agency. Human health evaluation manual, supplemental guidance: "Standard default exposure factors". OSWER Directive 9285.6-03.

Receptor Intake:

$$\text{Intake}_{i,j} := C_{\text{atm}}_{i,j} \cdot I$$

This is the receptor intake
in kg/s

0	0
0	0
$5.119 \cdot 10^{-10}$	$5.837 \cdot 10^{-10}$

$$C_{\text{atm}}$$

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